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Damien Gredat, Hugues Chaté, Ivan Dornic, Bertrand Delamotte. Finite-scale singularity in the renormalization group flow of a reaction-diffusion system. *Physical Review E: Statistical, Nonlinear, and Soft Matter Physics*, 2014, 89 (1), pp.10102. 10.1103/PhysRevE.89.010102 . cea-01384210

HAL Id: cea-01384210

<https://hal-cea.archives-ouvertes.fr/cea-01384210>

Submitted on 19 Oct 2016

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Finite scale singularity in the renormalization group flow of a reaction-diffusion system

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(Dated: November 7, 2012)

We study the nonequilibrium critical behavior of the pair contact process with diffusion (PCPD) by means of nonperturbative functional renormalization group techniques. We show that usual perturbation theory fails because the effective potential develops a nonanalyticity at a finite length scale: Perturbatively forbidden terms are dynamically generated and the flow can be continued once they are taken into account. Our results suggest that the critical behavior of PCPD can be either in the directed percolation or in a new (conjugated) universality class.

Reaction-diffusion systems involving one particle species (also known as branching and annihilating random walks (BARW)) are stochastic out of equilibrium systems important from both a phenomenological and a theoretical viewpoint. They consist of identical particles A , diffusing on a d -dimensional lattice, that can branch ($nA \rightarrow (n+p)A$) or annihilate ($nA \rightarrow (n-q)A$). The competition between these two types of reaction is generically responsible for the existence of transitions between an active phase where the density of particles is finite, and an “absorbing” phase where all particles, and thus all fluctuations, have disappeared. Such models provide the building blocks of a large variety of applications and models in physics and beyond, and are therefore of fundamental importance [1]. They also have the advantage of providing a relatively simple theoretical framework for the study of the different universality classes of absorbing phase transitions.

Our understanding of out-of-equilibrium critical phenomena in general and absorbing phase transitions in particular has benefited from perturbative approaches [5, 6], but important advances were brought recently by the application of nonperturbative renormalization group (NPRG) methods [2–4, 7]. For the two prominent cases of BARW, $A \rightarrow 2A$, $2A \rightarrow \emptyset$ which represents the directed percolation (DP) class, and $A \rightarrow 3A$, $2A \rightarrow \emptyset$ which belongs to the parity-conserving, or generalized voter class, the success of the NPRG owed to the presence of non-perturbative features.

The case of the “pair contact process with diffusion” (PCPD) has largely resisted analysis so far [8] but was not studied with NPRG methods. The simplest BARW model in this class consists of reactions $2A \rightarrow 3A$ and $2A \rightarrow \emptyset$ with rates σ and λ . (A limiting reaction such as $3A \rightarrow \emptyset$, with rate λ' , is actually needed to ensure a finite density active phase [32].) The distinctive feature of the PCPD is that two particles must meet to trigger branching. On general grounds, this is not expected to be a relevant ingredient defining universality classes, hence the interest raised by results obtained so far on the critical behavior of PCPD: It has been intensively stud-

ied numerically in $d = 1$ but remains unclear because of the presence of slow dynamics and/or strong corrections to scaling [13]. The debate, ongoing still recently, is to know whether PCPD belongs to the DP universality class [13–15] or not [16–19].

Even the status of d_c , the upper critical dimension of PCPD, is unclear: numerically, $d = 3$ seems beyond it [20], but in $d = 2$, the presence of large corrections to scaling is difficult to disentangle from logarithmic terms preventing clear conclusions in spite of indications of mean-field behavior [21, 22]. In perturbation theory the RG flow of PCPD goes to the Gaussian fixed point for $d > 2$ and sufficiently small coupling constants, whereas it blows up at a finite scale for larger couplings or for $d < 2$ [9]. This suggests $d_c = 2$. Note that the explosive flow forbids the exploration of the long-distance physics of the model. This is also known to occur in quantum chromodynamics (at the confinement scale), in the $O(N)$ nonlinear sigma model (at the scale of the correlation length) [10], and in pinned elastic manifolds (at the Larkin length) [11]. In this last case, NPRG methods at the functional level allowed to treat the problem [12].

In this Letter, we examine the PCPD field theory in the light of the NPRG, explain why perturbation theory fails, and how to avoid its problems. We show that the potential in the running effective action develops a singularity at a finite scale, signalling that couplings that are perturbatively forbidden are dynamically generated. Once taken into account the RG flow can be continued and a fixed point can be found. Our results suggest that the critical behavior of the model is either in the DP class or possibly in a new class characterized by a “conjugated” symmetry, and that $d_c = 2$ only at small coupling. Our study indicates that NPRG is a powerful tool for dealing with similar situations beyond reaction-diffusion systems.

The field theory associated with PCPD. By using the usual Doi-Peliti formalism [23] it is possible to derive the action associated with PCPD from first principles:

$$\mathcal{S} = \int_{\mathbf{x}} [\bar{\phi} (\partial_t \phi - D \nabla^2 \phi) + \phi^2 (g_1 \bar{\phi} + g_2 \bar{\phi}^2 + g_3 \bar{\phi}^3) + \phi^3 (3\lambda' \bar{\phi} + O(\bar{\phi}^2))] \quad (1)$$

where ϕ and $\bar{\phi}$ are complex conjugates, $\mathbf{x} = (t, \vec{x})$, $\int_{\mathbf{x}} = \int d^d x dt$, and $g_1 = 2\lambda - \sigma$, $g_2 = \lambda - 2\sigma$, $g_3 = -\sigma$. Within perturbation theory, one finds that initializing the RG flow with the (bare) couplings of the action \mathcal{S} , Eq.(1), the running coupling $g_2(k)$ (k being a momentum scale) diverges at a finite scale k_c for $d < 2$ which bars from exploring scales below k_c . Moreover, the $\langle \phi \phi \rangle$ response function does not receive any loop correction and thus the dynamical exponent z remains equal to 2 which is clearly invalidated by numerical results. For $d > 2$, all couplings are irrelevant around the Gaussian fixed point which is thus (locally) attractive. (Hence the conclusion that $d_c = 2$.) We now present a calculation where the flow no longer diverges but develops a singularity that can naturally be taken into account at the price of working functionally.

The nonperturbative renormalization group. NPRG follows Wilson's idea [24] of partial integration over fluctuations. It builds a one-parameter family of models indexed by a momentum scale k such that fluctuations are smoothly included as k is lowered from the inverse lattice spacing Λ down to $k = 0$ where they have all been summed over. To this aim, we add to the original action a momentum-dependent mass-like term [25, 26]

$$\Delta \mathcal{S}_k = \frac{1}{2} \int_{\mathbf{q}} \phi_i(-\mathbf{q}) [R_k(q)]_{ij} \phi_j(\mathbf{q}) \quad (2)$$

where $\mathbf{q} = (\omega, \vec{q})$, $q = |\vec{q}|$, $i = 1, 2$, $\phi_1 = \phi$, $\phi_2 = \bar{\phi}$ and repeated indices are summed over. With, e.g., $[R_k]_{12} = [R_k]_{21} = (k^2 - q^2)\theta(k^2 - q^2)$ and $[R_k]_{11} = [R_k]_{22} = 0$, the fluctuation modes $\phi_i(q > k)$ are unaffected by $\Delta \mathcal{S}_k$ while the others with $q < k$ are essentially frozen. The k -dependent generating functional of correlation and response functions thus reads

$$\mathcal{Z}_k[J_1, J_2] = \int D\phi D\bar{\phi} e^{-S - \Delta \mathcal{S}_k + \int_{\mathbf{x}} J_i \phi_i}. \quad (3)$$

The effective action $\Gamma_k[\psi_i]$, where $\psi_1 = \psi = \langle \phi_1 \rangle$, $\psi_2 = \bar{\psi} = \langle \phi_2 \rangle$, is given by the Legendre transform of $\mathcal{W}_k = \log \mathcal{Z}_k$ (up to the term proportional to R_k):

$$\Gamma_k[\psi, \bar{\psi}] + \mathcal{W}_k = \int_{\mathbf{x}} J_i \psi_i - \int_{\mathbf{q}} R_k(q) \psi(\mathbf{q}) \bar{\psi}(-\mathbf{q}). \quad (4)$$

The two-point functions can be computed from Γ_k by differentiating:

$$[\Gamma_k^{(2)}]_{i_1 i_2}[\mathbf{x}_1, \mathbf{x}_2, \psi, \bar{\psi}] = \frac{\delta^2 \Gamma_k}{\delta \psi_{i_1}(\mathbf{x}_1) \delta \bar{\psi}_{i_2}(\mathbf{x}_2)} \quad (5)$$

and the exact flow equation for $\Gamma_k[\psi, \bar{\psi}]$ reads [25]:

$$\partial_k \Gamma_k = \frac{1}{2} \text{Tr} \int_{\mathbf{q}} \partial_k R_k \cdot G_k \text{ with } G_k = [\Gamma_k^{(2)} + R_k]^{-1}. \quad (6)$$

When k decreases from Λ to 0, Γ_k varies between the (bare) action: $\Gamma_{k=\Lambda} = \mathcal{S}$, and the full effective action:

$\Gamma_{k=0} = \Gamma$. Solving the flow equation (6) is thus equivalent to solving the model. This is however impossible to do exactly and approximations must be made. We perform here the local potential approximation (LPA) which is known to work well for the determination of the critical behavior of models either at equilibrium or out-of-equilibrium [2, 3, 25, 27]:

$$\Gamma_k \rightarrow \Gamma_k^{\text{LPA}} = \int_{\mathbf{x}} (\bar{\psi}(\partial_t - D\nabla^2)\psi + U_k(\psi, \bar{\psi})). \quad (7)$$

Substituting Eq.(7) into Eq.(6), choosing the R_k function described above and integrating over \mathbf{q} , we find :

$$\partial_k U_k = C_d \left[\frac{k^2 + U_k^{(1,1)}}{\sqrt{(k^2 + U_k^{(1,1)})^2 - U_k^{(0,2)} U_k^{(2,0)}}} - 1 \right] \quad (8)$$

where $C_d = 4k^{2+d}[2^{d+1}\pi^{d/2}d\Gamma(d/2)]^{-1}$ and the upper indices code for derivatives in ψ and $\bar{\psi}$. It is easy to verify that performing a field expansion of $U_k(\psi, \bar{\psi})$ around $(0, 0)$ leads, for the couplings in front of the monomials $\psi^m \bar{\psi}^n$, to the same difficulties as encountered perturbatively: the flow blows up at a finite scale for $d < 2$. We thus need to work functionally. However, we can further simplify our ansatz Eq.(7) by performing an expansion of $U_k(\psi, \bar{\psi})$ in $\bar{\psi}$ only while remaining functional in the ψ -direction. We thus replace $U_k(\psi, \bar{\psi})$ by

$$U_k(\psi, \bar{\psi}) \rightarrow \sum_{n=1}^N \bar{\psi}^n V_{n,k}(\psi) \quad (9)$$

and we typically truncate the sum at order $N = 3$ or 4. Our approximation scheme is therefore based on the assumption that the LPA is sufficient, and that the non-trivial features of the model lie in the ψ direction (which is not spoiled by the expansion in $\bar{\psi}$). Inserting Eq.(9) into Eq.(8) we find the flow equations for the functions $V_{n,k}$ at order $N = 3$:

$$\dot{V}_1 = B V_2 V_1'' \quad (10)$$

$$\dot{V}_2 = B \left[\frac{1}{2} V_1'' (A V_2 (3 A V_2 V_1'' - 8 V_2') + 6 V_3) + V_2 V_2'' \right] \quad (11)$$

$$\begin{aligned} \dot{V}_3 = B \left[\frac{1}{2} (A (8 V_2' (3 V_1'' (A V_2 V_2' - V_3) - V_2 V_2'')) \right. \\ \left. + V_2 V_1'' (A (V_1'' (A V_2 (5 A V_2 V_1'' - 24 V_2') + 18 V_3) \right. \\ \left. + 6 V_2 V_2'') - 12 V_3')) + 6 V_3 V_2'' \right) + V_2 V_3'' \right] \quad (12) \end{aligned}$$

where, for simplicity, we have omitted the index k in the functions $V_{n,k}$, V_n' and V_n'' are the derivatives of these functions with respect to ψ , $\dot{V}_n = k \partial_k V_n$, $A = (k^2 + V_1')^{-1}$ and $B = (k^{d+2} 4 v_d / d) A^3 |A^{-1}|$. The initial conditions of these flow equations are provided by the action \mathcal{S} with

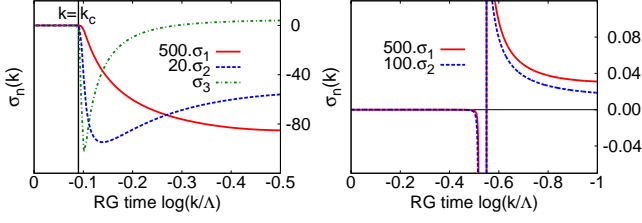


FIG. 1: (color online) Left: Flows in $d = 1$ of the linear couplings $\sigma_n(k) = V'_{n,k}(0)$ in the semi-functional approach, Eq.(9). Right: Same when U_k is expanded in both ψ and $\bar{\psi}$ and infinitesimal linear couplings are considered ($\sigma_1(k = \Lambda) = 0$, $\sigma_2(k = \Lambda) = 10^{-8}$, all other rates are of order 1). Only terms at most quartic in the fields have been retained. The RG flow of all couplings remains finite but shows an abrupt change around $k_c \simeq 0.6$.

$\phi_i \rightarrow \psi_i$. They impose that $\forall n: V'_{n,k=\Lambda}(\psi = 0) = 0$: the bare potential has no linear term in ϕ . Perturbatively, it is easy to show that these terms cannot be generated in U_k since all Feynman diagrams involve at least two incoming particles and thus two fields ψ .

We have numerically integrated the coupled flow equations of the functions $V_{n,k}(\psi)$ with $N = 4$ (see Eqs.(10) for the $N = 3$ case) together with the initial conditions provided by \mathcal{S} , Eq.(1). In the early stage of this flow, the linear term of each of these functions remains identically zero as naively expected. However, at a finite scale k_c which is typically the scale where the perturbative flow blows up, a linear term is generated in all these functions (Fig.1): the potential U_k develops a *corner* at $\psi = 0$ and its analytic structure is changed below k_c .

A detailed study of the emergence of the linear terms reveals that for $k \gtrsim k_c$, a boundary layer appears in the $V_{n,k}(\psi)$ functions such that in the inner part of the layer, that is, at small ψ , these functions are expandable around $\psi = 0$ (for $\psi \geq 0$) and start quadratically in ψ . In the outer region, a linear part appears in the $V_{n,k}(\psi)$ functions. As k approaches k_c from above, the width of the layer decreases and vanishes at k_c , leaving the linear term as the dominant term around $\psi = 0$ (Fig.2). Below k_c , the linear terms remain present in the vicinity of $\psi = 0$ and the flow can be continued all the way to $k = 0$. We have checked that this emerging scenario holds at order $N = 3$ and 4 of the $\bar{\psi}$ -expansion. Converged, higher-order results are unfortunately difficult to obtain [33].

We have confirmed our scenario by considering the usual set of reactions $2A \rightarrow 3A$, $2A \rightarrow \emptyset$ and $3A \rightarrow \emptyset$ complemented by $A \rightarrow 2A$ and $A \rightarrow \emptyset$ with infinitesimal rates. Expanding the potential U_k in both ψ and $\bar{\psi}$ we now have (at least) two new couplings that are linear in ψ : $\sigma_1(k)\psi\bar{\psi}$ and $\sigma_2(k)\psi\bar{\psi}^2$ with $\sigma_{1,2}(k = \Lambda)$ infinitesimal. If the limit $\sigma_{1,2}(k = \Lambda) \rightarrow 0$ were regular then $\sigma_{1,2}(k)$ would start playing a significant role in the RG flows of the other couplings only below a very small scale k that would go to 0 as $\sigma_{1,2}(k = \Lambda) \rightarrow 0$. We find on

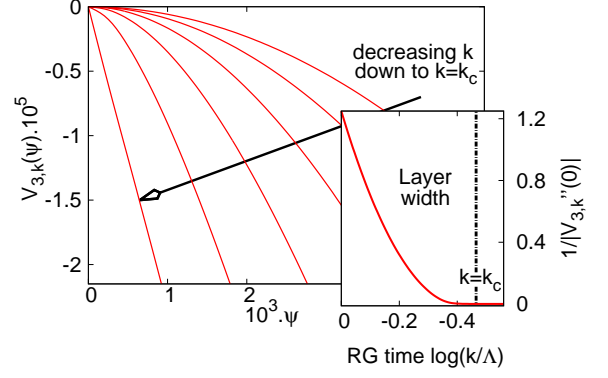


FIG. 2: (color online) Boundary layer for $V_{3,k}(\psi)$, whose behavior around the origin is displayed for $k \simeq k_c$ and several values of k above k_c . For all $k > k_c$, $V_{3,k}$ starts quadratically at $\psi = 0$ whereas a linear term appears at $k = k_c$. Inset: width of the boundary layer as a function of $\log k/\Lambda$.

the contrary that while for k just below Λ the flows of all the couplings are indeed almost insensitive to $\sigma_{1,2}$ (when they are initially extremely small), this is no longer the case for $k \simeq k_c$ since the dramatic increase of $g_2(k)$ makes $\sigma_{1,2}(k)$ grow abruptly around k_c , independently of their initial smallness, see Fig. 1. For k close to k_c , the back reactions of $\sigma_{1,2}(k)$ on the flows of all the other couplings start to be significant and eventually modify them completely since $\sigma_{1,2}$ are the most relevant couplings. The RG flow is no longer singular ($g_2(k_c)$ remains finite) but lives below k_c in a larger functional space involving the couplings linear in ψ . This result is fully consistent with what is found in the functional viewpoint.

Criticality in $d = 1$. Our two different approaches both conclude that terms linear in ψ are generated below a nonuniversal scale k_c in $d = 1$. We can therefore consider the field theory obtained just below k_c as a new field theory that can be studied per se, the difficulty being that its action is non polynomial since the functions $V_{n,k}(\psi)$ are not. In a perturbative analysis only the terms of lowest degrees in ψ and $\bar{\psi}$ would be retained in the bare action, *i.e.* $\psi\bar{\psi}$, $\psi^2\bar{\psi}$ and $\psi\bar{\psi}^2$. Depending on the relative sign of the two cubic terms, this action, truncated at order three, exhibits one of the following symmetries (after a trivial rescaling of the fields): $\bar{\psi}(t) \rightleftharpoons \pm\psi(-t)$. The minus sign corresponds to the cubic terms having opposite signs. This is the “rapidity” symmetry defining the DP class. The other sign defines a new, “conjugated”, symmetry. We call the corresponding class DP’. It is easy to show in our framework, Eq.(8), that when only the above terms are kept in U_k , only two nontrivial fixed points exist and that they show either one or the other of the above symmetries (we call them DP and DP’). No such result exists beyond this simple truncation. To the best of our knowledge, the DP’ symmetry has never

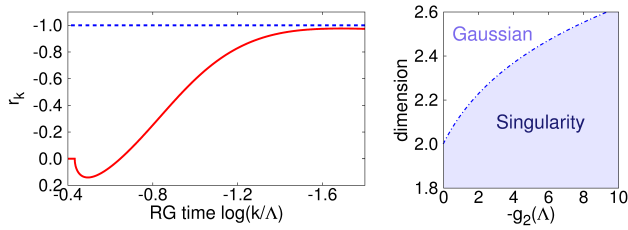


FIG. 3: (color online) Left: Flow of the symmetry-testing ratio r_k computed in the semi-functional approach with $N = 4$. For $k < k_c$, r_k flows toward the DP value $r_k^{(DP)} = -1$. Right: line separating the basin of attraction of the Gaussian fixed point and the domain where the singularity is present in the $(d, g_2(\Lambda))$ plane when $g_1(\Lambda) = 0$.

appeared nor been studied before.

Two difficulties appear when studying the existence and the nature of the fixed point. First, when using a complete field expansion of U_k , it is difficult to initialize the flow below k_c with what has been found functionally using Eq.(9) just after the singularity because this amounts to projecting functions of ψ onto polynomials, setting infinitely many terms of high degree to 0. Second, if we work directly with our semi-functional approximation, Eq.(9), the roles of ψ and $\bar{\psi}$ are dissymmetric which hinders the search of a fixed point exhibiting a symmetry that exchanges ψ and $\bar{\psi}$ as in DP or DP'. We have nevertheless studied the existence of a fixed point using both approaches. Within richer and richer polynomial approximations of U_k (where ψ and $\bar{\psi}$ play symmetric roles) initialized with couplings found with the semi-functional approximation just after the singularity, we have found a range of initial reaction rates leading to the DP fixed point. In the other, semi-functional approximation truncated at order $N = 4$, we have recorded the flow of $r_k = (U_k^{(2,1)}/U_k^{(1,2)})\sqrt{U_k^{(1,3)}/U_k^{(3,1)}}$ (calculated at $\psi = \bar{\psi} = 0$). This quantity is an indicator of the nature of the fixed point because if $r_k = -1$ the expansion of U_k up to order four in the fields exhibits the rapidity symmetry (up to a rescaling of the fields). If $r_k = +1$ the same holds true for the DP' symmetry. Notice that just below k_c , r_k is neither 1 nor -1 . We show in Fig.3 the evolution of r_k computed from Eq.(9) with $N = 4$. Although the instabilities of our numerical code prevent us from finding a true fixed point value for r_k there is little doubt that it indeed reaches a plateau at the value -1 so that the expected fixed point should be that of DP in agreement with what is found in the polynomial approximation. Notice however that if we work with a field truncation of U_k , starting at $k = \Lambda$ with a very small coupling $\sigma_2(k = \Lambda)$ as explained above, we find, at least in the simplest truncation of U_k , either the DP or DP' fixed points depending on the initial rates (we have not been able to confirm this result with truncations involving higher powers of the fields because of the extreme

sensitivity of the flow at small k on the choice of the initial rates). Interestingly, we find that the vicinity of both fixed points is reached after a very long RG “time” ($\log k/\Lambda \sim -9$) which means that the scaling regime only appears at very large lengthscales. This could explain why it is so difficult to observe the asymptotic regime in numerical simulations. Our general conclusion is therefore that the critical behavior of PCPD in $d = 1$ should be either in the DP or DP' universality class and our best results are in favor of DP.

The upper critical dimension. The determination of d_c is the same in perturbation theory and in our scheme for small initial couplings: for $d > 2$, the conditions $g_{1,\Lambda} = 0$ and $g_{2,\Lambda}$ small make the system critical and the flow is driven towards the Gaussian fixed point. However, for large enough $g_{2,\Lambda}$ the flow always becomes singular, even when $g_{1,\Lambda} = 0$. We show in Fig.3 the basin of attraction of the Gaussian fixed point in this case as a function of $g_{2,\Lambda}$ obtained within perturbation theory. The result is similar to what is found in the Kardar-Parisi-Zhang equation [28][34]. Note that within perturbation theory, criticality is reached when $g_{1,\Lambda} = 0$. It is no longer clear in our approach that this condition is necessary for large initial $g_{2,\Lambda}$ and $d > 2$ because the finite scale singularity emerges for generic $g_{1,\Lambda}$. Our results suggest that there could exist a nontrivial critical behavior at large initial $g_{2,\Lambda}$ even above one dimension that could be in the DP (or possibly DP') universality class.

To conclude, we believe our results represent a breakthrough for the understanding of the critical behavior of PCPD. Even though we do not have yet a complete solution of the problem, we have unlocked an heretofore blocked situation and offered new lines of further research. The recourse to functional nonperturbative renormalization was essential because it allows us to address questions such as the generation of linear terms. Going beyond our semi-functional approximation remains the main challenge that should lead, once controlled numerically, to satisfactory results. From a physical point of view, a final answer to the question of the phase diagram and its accessible fixed points in all dimensions remains of course the main goal. But understanding the meaning of the scale k_c is also challenging. It could be related to the existence of relevant “elementary excitations” made of pairs of particles that would involve an intrinsic scale. Disentangling the roles of the particles and of the pairs has already been studied by effectively taking them into account through the introduction of another species B and the reactions: $2A \rightarrow B$, $B \rightarrow A$, $B \rightarrow 2B$, $2B \rightarrow B$, $B \rightarrow \emptyset$. Such two-species PCPD models, which are believed to exhibit the same critical behavior as the one species case studied here [31], could be the starting point of more complicated NPRG approaches (involving four fields, but possibly deprived of singularities in the flow). These endeavors are left for future work.

We thank Matthieu Tissier and Gilles Tarjus for illuminating discussions.

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